Quantum interferences in the photodissociation of $Cl_2(B)$ in superfluid helium nanodroplets $(^4He)_N$

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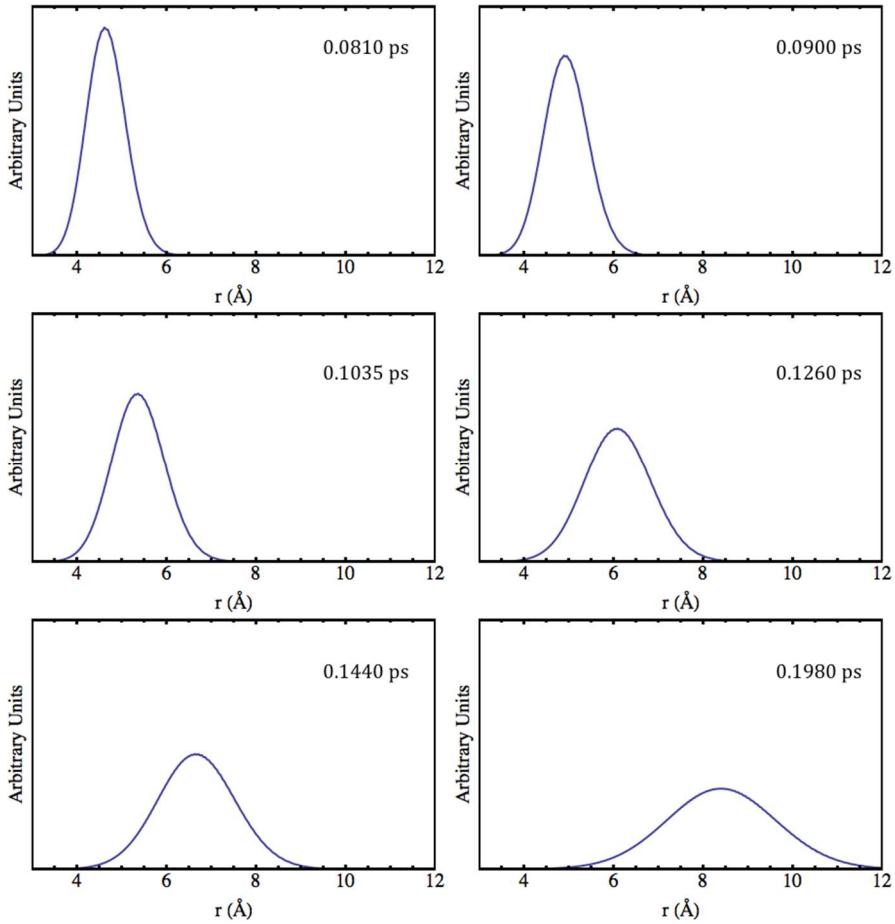
Supplementary Information

Table S1. Initial values of the energies (in K) involved in the process.

N	E_{Kin} Cl_2(B)	E_{Pot} Cl_2(B)	$E_{Interac.}$ Cl_2(B)-helium	E_{Kin} helium	$E_{Pot+Corr}$ helium
50	199.1	11094.1	-345.9	202.6	-125.6
100	199.2	11094.1	-388.7	254.0	-380.3
200	199.2	11094.1	-410.1	287.8	-902.4
300	199.3	11094.1	-416.8	306.1	-1447.5
500	199.3	11094.1	-421.5	330.4	-2580.7

a



b

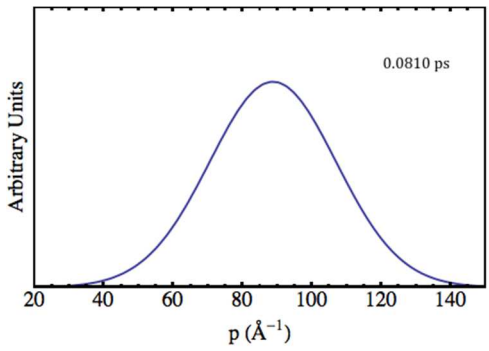


Figure S1. (a) Snapshots of the squared modulus of the Cl_2(B) relative coordinate wave packet in gas phase. (b) The same as in (a) but for the wave packet in momentum representation; in this case the results for the other times are coincident with that for the smallest one (*t*=0.0810 ps).

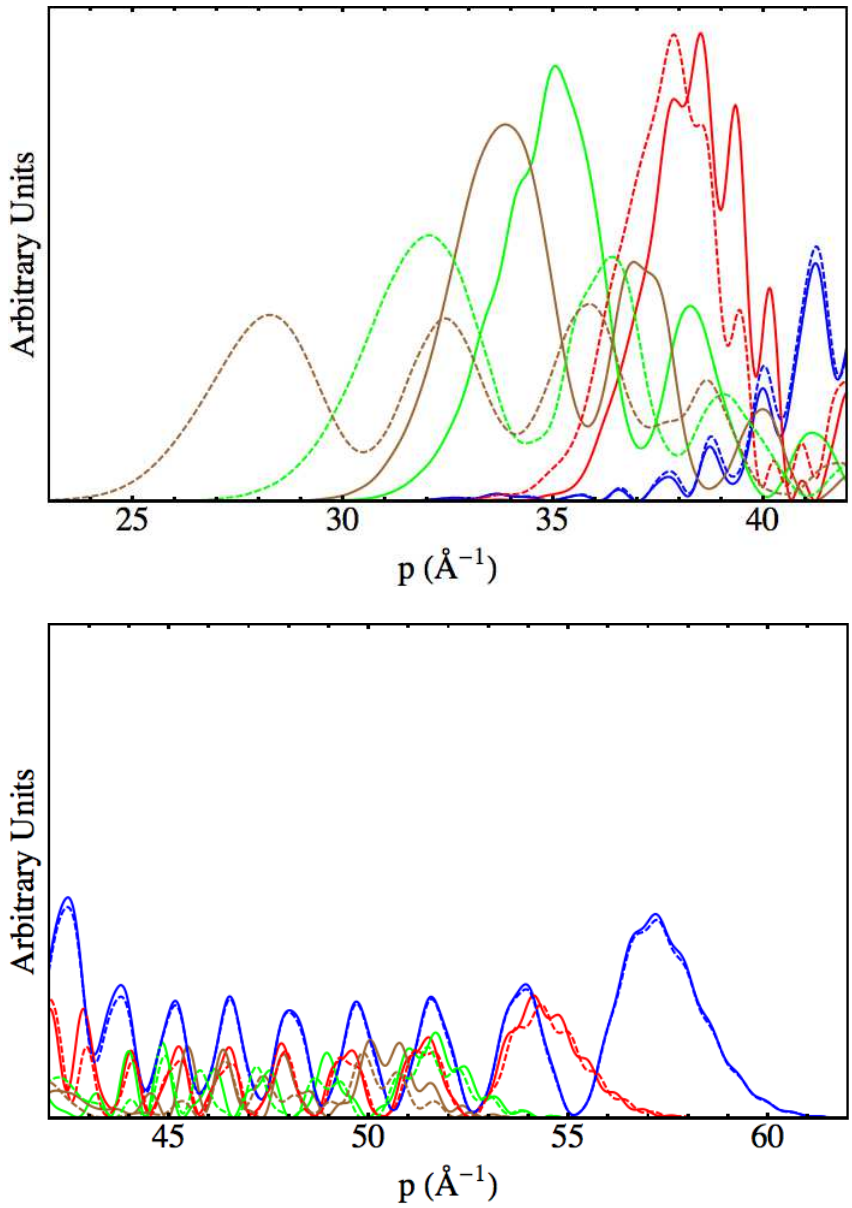


Figure S2. Squared modulus of the Cl_2(B) wave packet in momentum representation, given in more detail than in Figure 4 (up), at some time values for which the Cl atoms are travelling inside the nanodroplet [*t*(ps) = 0.657 (blue), 0.918 (red), and 1.202 (green)] and when they are relatively close to the nanodroplet surface [*t*(ps) = 1.346 (brown)]. Low-intermediate p values (up) and intermediate-high p values (down). Two nanodroplet sizes are considered: *N*=300 (continuous line) and *N*=500 (dashed line).

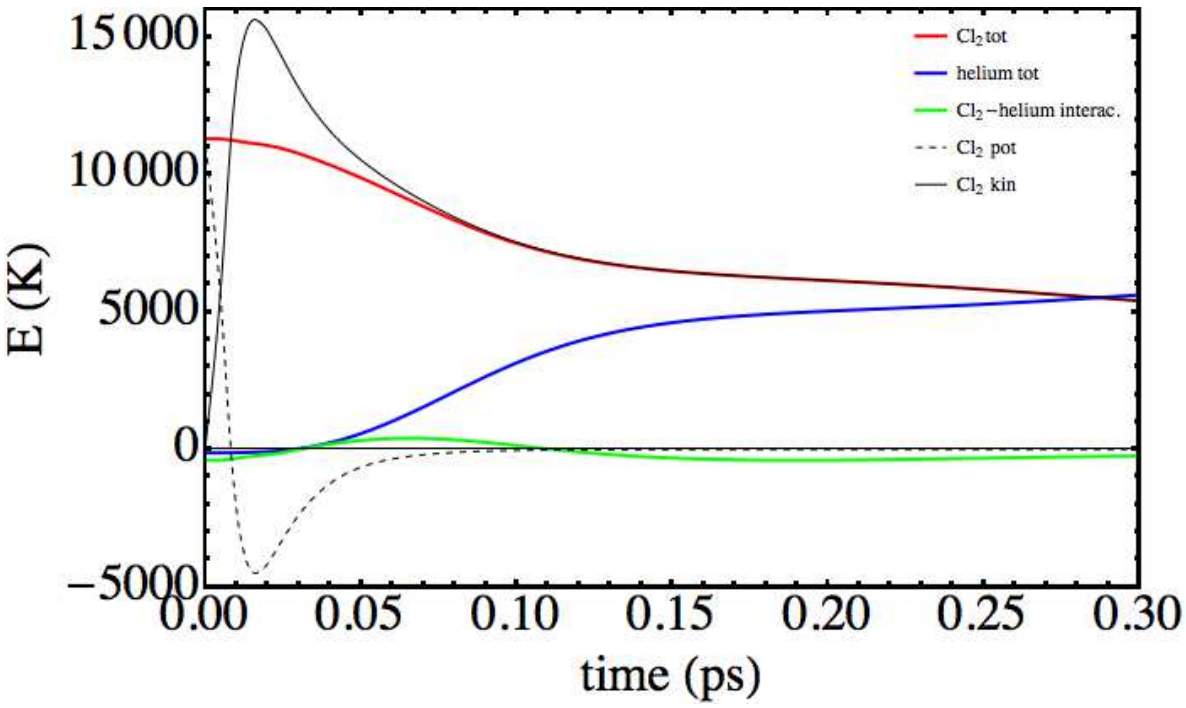


Figure S3. Time evolution of the energies involved in the process: Cl_2(B) total energy (Cl-Cl potential + kinetic), solid red line; helium total energy (helium potential+correlation + kinetic), solid blue line; Cl_2(B)-helium interaction, solid green line; Cl_2(B) potential energy, dotted black line; Cl_2(B) kinetic energy, solid black line. The values reported are for N = 100, but at the early times of the photodissociation the same trends are found for all nanodroplets.

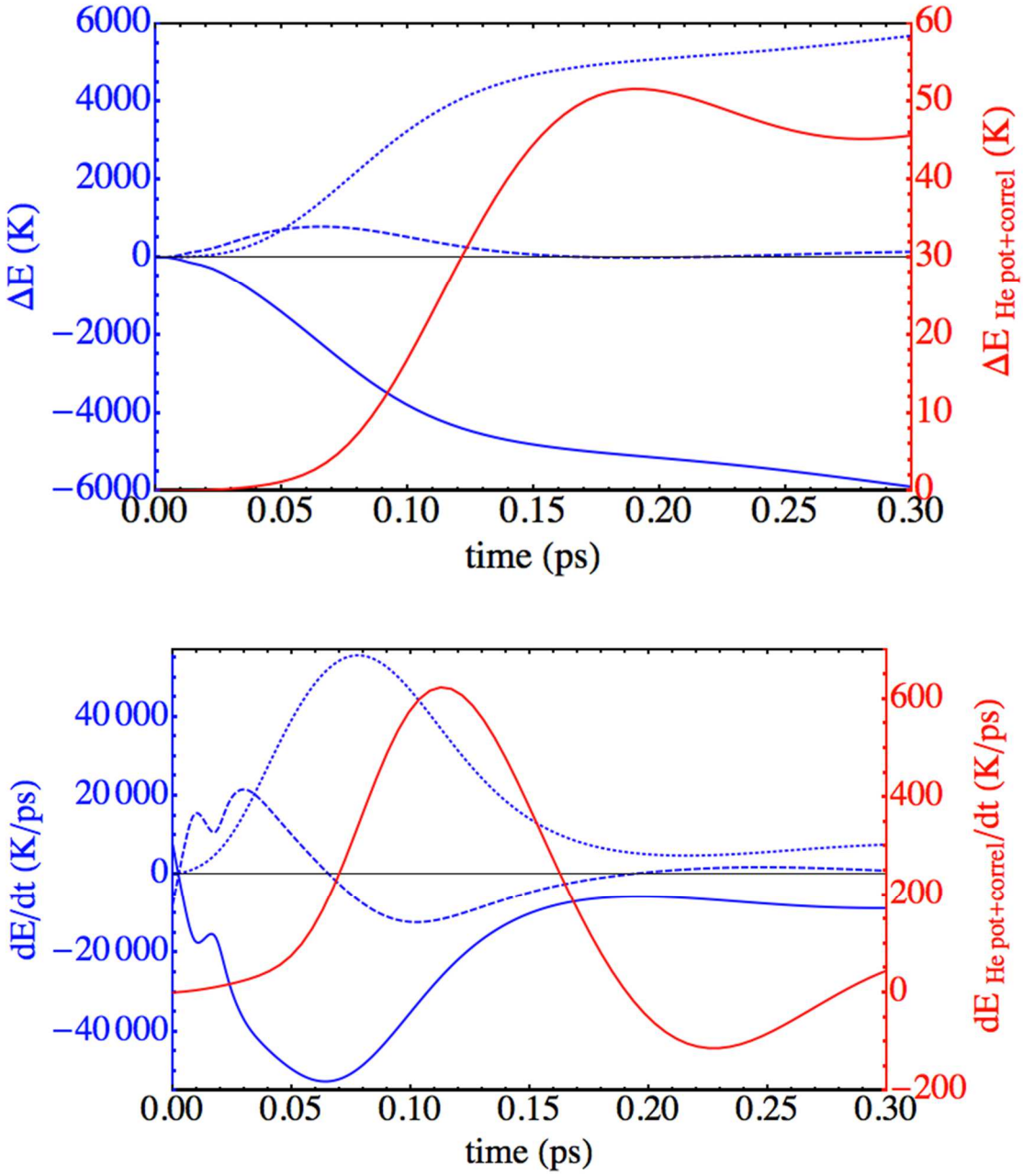


Figure S4. Time evolution of the change of Cl_2(B) kinetic+potential energy (solid blue line), Cl_2(B)-helium interaction energy (dashed blue line), helium internal kinetic energy (dotted blue line), and helium internal potential+correlation energy (red) for the initial time period of the photodissociation (up). Evolution of the time derivatives of the former quantities, i.e., their rates of change (down). The values reported are for N = 100.

Movie 1. Time evolution of the squared modulus of the Cl_2(B) wave packet in coordinate representation (blue) and effective potential (red), during part of the photodissociation process (0.0-3.0 ps time interval), for the [Cl_2(B)@(^{4}He)$_{500}$]* nanodroplet. In this case the time required for <r> to be equal to the diameter of the nanodroplet is ≈ 2.6 ps. See the AVI video file "movie 1 WP(r)^2 N=500.avi" (5.41 MB).

Movie 2. Time evolution of the squared modulus of the Cl_2(B) wave packet in momentum representation (blue), during part of the photodissociation process (0.0-3.0 ps time interval), for the [Cl_2(B)@(^{4}He)$_{500}$]* nanodroplet. See the AVI video file "movie 2 WP(p)^2 N=500.avi" (4.78 MB).